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用**Kierlik-Rosinberg**的**DFT**方法研究活性炭分离空气中微量**CCl_4**

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摘要 以N_2作为空气的主要成分，利用Kierlik和Rosinberg提出的密度函数理论 (density functional theory, KR-DFT)研究了N_2/CCl_4双元混合物在活性炭内的 吸附。重点讨论了孔径、压力和温度对CCl_4 吸附选择性的影响，不为同条件下吸 附回收空气中的CCl_4提供了理论参考。在KR-DFT计算中。N_2 分子和CCl_4分子模 型化为单点的Lennard-Jones球；流体分子与吸附剂材料之间的作用采用平均场理 论中的10-4-3模型。在KR-DFT方法中，自由能采用标度的场粒子理论(scaled field particle theory, SPT)处理。讨论了孔径、压力和温度对吸附选择性的影 响。研究结果表明，常温下当空气中CCl_4的含量为1%时，1.39nm的孔径最有利于 CCl_4的吸附。

关键词 氮 四氯化碳 吸附剂 选择性 孔径

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Separation of CCl_4 from Air by Kierlik-Rosinberg's DFT Method on Activated Carbon

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Abstract The separation of binaiy mixture of N_2 and CCl_4 using activated carbon is studied by the new method of density functional theoiy proposed by Kierlik and Rosinberg. We discussed the effects of pore size, pressure and temperature on selectivity of CCl_4 for the N_2/CCl_4 mixtures. The study gave references of absorbing CCl_4 from air in diffei'ent condition. The nitrogen and CCl_4 molecules are modeled as Ixnnard-Jones spherical molecules, and the well-known Steele's 10-4-3 potential are used to represent the interaction between the fluid molecule and the solid wall. In DFT method, the Helmholtz free energy is dealt by ihe scaled field particle theory. The results indicate that the pore size of 1.39 nra is the ideal size to separate CCl_4 from air with molar fraction of 1 % .

Key words NITROGEN CARBON TETRACHLORIDE ADSORBENT SELECTIVITY PORE SIZE

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